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13. ABSTRACT *(Maximum 200 words)*

This work covers one of the basic computational issues in materials science, which is that of devising algorithms for computing microstructure. Finite element discretizations are used to approximate a standard energy density functional. Grid effects are found to affect the solutions in some cases and suitable remedies are investigated. Covolume methods are a second topic of research. Three dimensional error estimates are obtained. A new and optimal Voronoi-Delaunay mesh generator is given.

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FINAL TECHNICAL REPORT FOR AFOSR GRANT F49620-92-J-0133

Principal Investigator: Roy A. Nicolaides, Carnegie Mellon University

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PROGRESS AND ACHEIVEMENTS

1. Computational Methods for Microstructure

The development of numerical methods for solving problems in materials science is a subject which, with few exceptions, is in its infancy. This work covers one of the basic computational problems in the field which is that of devising algorithms for computing microstructures. Our efforts have all been directed towards computing the particular microstructures associated with martensitic phase transitions. Within this framework we have encountered both algorithmic and analytical problems, a number of which have been satisfactorily solved.

Our work addresses static problems. We are not currently able to handle full three dimensional time dependent cases. The typical stationary problem calls for the minimization of a highly nonconvex bulk energy functional. The extremizing functions are vector valued, representing displacement fields. The construction of the bulk energy functionals is a specialized task, depending on a detailed knowledge of the properties of materials. The functionals used in our work were derived by R. James, based on ideas of J. Ericksen. The functionals contain information about the structure of the crystal lattice and several material specific parameters. These functionals are relatively complex, being, for instance, eighth order polynomials in the displacements.

The research supported in the grant has addressed two main issues. The first issue concerns techniques for discretization of the bulk energy functionals and the second concerns algorithmic issues relevant to nonconvex optimization. In this we discovered some unusual and apparently paradoxical results. We will describe these results now.

As reported in [1] the initial discretization used bilinear finite elements in a planar model. In addition to the finite element approximation it is necessary to use some form of numerical integration to evaluate the energy since, as mentioned above it is a polynomial of high degree. Following the work of others, we used a midpoint quadrature approach combined with bilinear elements on a uniform square mesh. Minimizing the resulting function of the mesh variables (several thousand of them) leads in principle to the desired microstructure. Our important discovery here was that the 'microstructures' computed by others using this scheme are not microstructures at all, but are representations of numerical instabilities of the discretization technique. This situation occurs because both the microstructure and the numerical instability are manifested as grid scale oscillations. It can be hard to distinguish the two in many cases, but we constructed an example where there can be no doubt that the computed result represents the effect of numerical instability, although it has the physical appearance of a typical microstructure. The report [1] contains an explanation of the source of this instability and shows how to avoid it it certain cases. It seems unlikely that it can be avoided in general. If this is true it means that the original scheme is seriously flawed and we do, in fact, consider this to be the case.

To avoid the difficulties of the approach of the previous paragraph we decided to eliminate the integration errors entirely by the use of linear finite elements on triangles. This introduces another element of uncertainty in that with triangular meshes the grid orientation may play a role in the computed microstructure. Our experiences with this are reported in [2]. The major difficulty is that

when the mesh diagonals are not aligned with the microstructure they nevertheless are somehow able to 'capture' the microstructure and produce a result in which it is aligned with the mesh diagonals. This can occur even when the physical microstructure is meant to lie at 90 degrees to the mesh diagonals. The somewhat subtle reasons for the occurence of this phenomenon, explained in [2], are to be found in the existence of near minimizers in the energy sense which are far from the physical minimizers. At present, the only available solution to this difficulty is to compute on very fine meshes. Unfortunately, this is an expensive remedy. We have developed a theory to explain quantitatively how fine the mesh needs to be in particular cases and the techniques for this are presented in [2].

In the course of performing the computations of the two previous paragraphs a suprising effect of numerical optimization algorithms was noted. Specifically, when applied to nonconvex functionals, the usual descent algorithms can terminate at a saddle point of the functional rather than at a local minimum as would be expected. No warning of this situation is provided. It simply appears to the user that a minimum (local) has been found whereas in fact the computed solution is only a saddle point. We constructed a simple model to demonstrate this effect and provided some analysis of the character of the saddle point. This work is being written up for publication [3]. We are unsure how pervasive this phenomenon is likely to be in general, but we do have full scale microstructure computations in which it occurred.

The difficulties of computing microstructure in the form of grid scale oscillations are sufficiently great that it becomes of interest to seek alternative formulations. In one such formulation we seek averages of the oscillations rather than the oscillations themselves. A technique for this was proposed in our work [4]. We formulated an approach which is suitable for directly computing the Young measures which describe the mesh scale oscillations. The calculations in this case take place on a fixed mesh which is not unduly fine since the objects being computed are relatively slowly varying. One drawback of this approach is that since only averages are being found the microstructure must somehow be obtained from the averages. For design purposes however, the averages may be sufficient information. We had some success in computing with this approach in several different situations. However, there are more variables to keep track of and the optimization problem is a difficult one.

Beyond the purely computational issues, there is the question of assessing the theoretical accuracy of the computed solutions. The full microstructure problem is far too difficult for existing techniques. In fact, the underlying mathematical theory is not well developed for the particular problems of interest and so it is unwise to attempt to prove error estimates for these problems at present. Instead, we decided to see what can be said about simpler models. In one case, reported in [5] we were able to obtain rigorous results for a convexified problem. Our estimates are norm estimates and thus better than estimates in weak topologies.

2. Covolume techniques of discretisation

The covolume approach to discretization uses pairs of dual meshes to closely enforce physical laws at the discrete level. The technique is designed specifically around discretizing the vector field operators div, grad and curl and their various combinations. One big advantage of covolume discretizations is that vector identities such as div(curl)=0 and curl(grad)=0 have natural discrete analogs. In recent times, a solid theoretical framework has been built for these methods and they have been applied in several fields. We have made a number of contributions to this effort. In the current grant period we have made the contributions which are described below.

In [6] we present an error estimate for the covolume scheme for three dimensional div-curl problems

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on tetrahedral meshes in three dimensions. The three dimensional div-curl problem is a notoriously difficult one. It is overdetermined since it has four equations but only three dimensions. There are few, if any, discretizations which deal with the system directly. Usually, potentials or Biot-Savart integrals are used. Another indirect approach can be based on least squares although not without difficulty. On the other hand our algorithm provides a straightforward way to obtain a solution to such systems and the error estimate shows that the discretization is effectively optimal.

One problem with covolume methods is that unlike finite elements we do not have schemes of arbitrary order of accuracy for general meshes. As part of an effort to provide such schemes we have developed a higher covolume scheme for div-curl systems on regular meshes. This scheme is built on the standard scheme. Its accuracy is fourth order in the mesh spacing compared with second order for the standard scheme. We have a rigorous proof of the order of the scheme. This is reported in [7]. The algorithm is equally applicable in two and three dimensions. However, we have no yet succeeded in extending it to triangular and tetrahedral meshes in any concise way. If this were possible, the resulting scheme would most likely be third order as opposed to first order for the standard scheme.

As mentioned previously, covolume schemes use dual mesh systems. The prototypical such mesh pair is a Voronoi-Delaunay system. These meshes have numerous applications in computational geometry and have been used as finite element meshes for a number of years. Their use in the covolume scheme is associated with the geometrical property that the edges of the Voronoi diagram are orthogonal to the faces of the Delaunay triangulation (or tesselation) and reciprocally. The usual situation envisages a convex domain to be triangulated, but of course this is insufficient for partial differential equations where restrictions on geometries cannot be tolerated. For this reason we have developed a new algorithm for making Voronoi-Delaunay mesh systems for arbitrary domains. Our new algorithm is based on correlating a set of nodes to a uniform mesh. (The uniform mesh is used as a tool for forming the Voronoi-Delaunay system. It has nothing to do with the discretization itself.) We have been able to show that our algorithm is optimal in time and space. It is highly suitable for partial differential application having a number of local properties. For instance, we know ahead of time how many and which elements have to be changed when a new point is added. This work is reported in [8].

In [10] we presented a comprehensive covolume scheme for the compressible Navier-Stokes equations. The book [9] which we assembled and edited contains a survey article for covolume algorithms generally.

CUMULATIVE PUBLICATIONS

[1] Austenite-Martensite computations avoiding spurious oscillations:(with D. Kinderlehrer and H. Wang) in Proceedings of the 1993 North American Conference on Smart Materials and Structures, SPIE Publications

[2] Mesh orientation and capturing effects in microstructure computations:(with N. Walkington and H. Wang) (will be submitted to SIAM Journal on Scientific and Statistical Computing)

[3] Spurious saddle point optimizers in nonconvex variational problems: (in preparation)

[4] Computation of microstructure utilizing Young's measure representations:(with N. Walkington) Journal of Intelligent Materials, Systems and Structures Vol4, No. 4, 1993

[5] Finite element estimates for Young's variational problem:(with N. Walkington) (to appear in Mathematics of Computation)

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[5] Finite element estimates for Young's variational problem:(with N. Walkington) (to appear in Mathematics of Computation)

[6] Covolume estimates for three dimensional div-curl systems:(with X. Wu) (will be submitted to SIAM Journal of Numerical Analysis)

[7] A fourth order staggered mesh technique for planar div-curl systems:(with D. Wang) (will be submitted to Numerische Mathematik)

[8] A Voronoi Delaunay mesh generator and its application to nonconvex domains:(with W. Rieder) (in preparation)

[9] Incompressible Computational Fluid Dynamics: (Book edited jointly with M. D. Gunzburger) Cambridge University Press, 1993

[10] Three dimensional covolume algorithms for viscous flow: Chapter 10 of Algorithmic Trends in Computational Fluid Dynamics, ed. M. Hussaini et al. Springer-Verlag 1993

GRADUATE STUDENTS SUPPORTED

William RIeder, a graduate student in the Department of Mathematics, Carnegie Mellon University was supported during the reporting period. Mr Rieder is expected to obtain his Ph. D. in August 1994.

Christopher Dalton, a graduate student in the Department of Mathematics, Carnegie Mellon University was supported during the reporting period.

INVITED PRESENTATIONS

10-4-1992 University of Pittsburgh, Pennsylvania: Three Rivers Conference on Applied Mathematics

5-5-1992 Virginia Polytechnic Institute, Blacksburg, Virginia: Conference on Smart Materials

7-1-1992 Cambridge University, England: Joint AMS-LMS Meeting, Numerical Analysis of Nonlinear Problems

7-1-1992 Cambridge University, England: Joint AMS-LMS Meeting, Computational Methods for Materials Science

6-8-1993 Carnegie Mellon University: 11th Army Conference on Applied Mathematics and Computing

11-3-1993 Brown University, Providence, Rhode Island: College Colloquium

12-14-1993 ICASE, NASA Langley Research Center, Hampton, Virginia: Colloquium

3-31-1994 University of Arkansas, 18th Annual Lecture Series in the Mathematical Sciences